Tandem Cofacial Stacks of Porphyrin-Phthalocyanine Dyad through Complementary Coordination

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1. NMR Measurements:

**Figure S1.** $^1$H NMR (600 MHz) spectrum of H$_2$(ImP)-Zn(nBuO)$_6$Pc in CDCl$_3$ at 25 °C.

**Figure S2.** $^{13}$C NMR (150 MHz) spectrum of H$_2$(ImP)-Zn(nBuO)$_6$Pc in CDCl$_3$ at 25 °C.
Figure S3. $^1$H-$^1$H COSY spectrum of H$_2$(ImP)-Zn(nBuO)$_6$Pc in CDCl$_3$ at 25 °C.
Figure S4. \(^1\)H-\(^1\)H ROESY spectrum of H\(_2\)(ImP)-Zn(nBuO\(_6\)Pc) in CDCl\(_3\) at 25 °C.

Figure S5. \(^1\)H-\(^{13}\)C HMOC spectrum of H\(_2\)(ImP)-Zn(nBuO\(_6\)Pc) in CDCl\(_3\) at 25 °C.
Figure S6. $^1$H-$^{13}$C HMBC spectrum of H$_2$(ImP)-Zn(nBuO$_6$Pc) in CDCl$_3$ at 25 °C.

Figure S7. $^1$H NMR (600 MHz) spectrum of H$_2$(ImP)-Zn(nBuO$_6$Pc) with 10% TFA in CDCl$_3$ at 25 °C.
**Figure S8.** $^1$H NMR (600 MHz) spectrum of H$_2$(ImP)-Zn(tBu$_3$Pc) in CDCl$_3$ at 25 °C.

**Figure S9.** $^{13}$C NMR (150 MHz) spectrum of H$_2$(ImP)-Zn(tBu$_3$Pc) in CDCl$_3$ at 25 °C.
Figure S10. $^1$H-$^{13}$C HMOC spectrum of H$_2$(ImP)-Zn(tBu$_3$Pc) in CDCl$_3$ at 25 °C.
2. Spectral Titration:

Figure S11. Spectral titration of H₂(ImP)-Zn(tBu₃Pc) with 1-methylimidazole (recorded on addition of every 5000 equivalent of 1-methylimidazole up to 150000 equivalent, and then 200000, 300000, 400000, and 500000 equivalent) in toluene at 25 °C. Fluorescence spectra were shown normalized at excitation wavelength at 455 nm (recorded on every observation of absorption spectra).

Figure S12. Spectral titration of H₂(ImP)-Zn(tBu₃Pc) with 1-methylimidazole (recorded on addition of every 5000 equivalent of 1-methylimidazole up to 150000 equivalent) in THF at 25 °C. Fluorescence spectra were shown normalized at excitation wavelength at 455 nm (recorded on addition of every 50000 equivalent of 1-methylimidazole).
**Figure S13.** Spectral titration of $\text{H}_2(\text{ImP})\cdot\text{Zn(}t\text{Bu}_3\text{Pc)}$ with 1-methylimidazole (recorded on addition of every 1000 equivalent of 1-methylimidazole up to 6000 equivalent) in $\text{CH}_2\text{Cl}_2$ at 25 °C. Fluorescence spectra were shown normalized at excitation wavelength at 455 nm (recorded on addition of 0 and 6000 equivalent of 1-methylimidazole).

**Figure S14.** Spectral titration of $\text{H}_2(\text{ImP})\cdot\text{Zn(}n\text{BuO}_6\text{Pc)}$ with 1-methylimidazole (recorded on addition of every 5000 equivalent of 1-methylimidazole up to 150000 equivalent) in toluene at 25 °C. Inset shows the fitting plot for absorbance at 717 nm. Fluorescence spectra were shown normalized at excitation wavelength at 455 nm (recorded on addition of every 5000 equivalent of 1-methylimidazole up to 150000 equivalent).
Figure S15. Spectral titration of $\text{H}_2(\text{ImP})\text{-Zn(nBuO}_6\text{Pc})$ with 1-methylimidazole (recorded on addition of every 5000 equivalent of 1-methylimidazole up to 150000 equivalent) in THF at 25 °C. Fluorescence spectra were shown normalized at excitation wavelength at 455 nm (recorded on addition of 0, 100000, 150000, 200000, and 250000 equivalent of 1-methylimidazole, and the spectrum without 1-methylimidazole was magnified by 10 times).

Figure S16. Spectral titration of $\text{H}_2(\text{ImP})\text{-Zn(nBuO}_6\text{Pc})$ with 1-methylimidazole (recorded on addition of every 1000 equivalent of 1-methylimidazole up to 6000 equivalent) in $\text{CH}_2\text{Cl}_2$ at 25 °C. Fluorescence spectra were shown normalized at excitation wavelength at 455 nm (recorded on addition of 0 and 6000 equivalent of 1-methylimidazole).